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Constrained State and Unknown Input Estimation for Nonlinear Singular Systems Using an URNDDR Approach

Shuwen Pan, Hongye Su, Pu Li*, and Yong Gu

Abstract— **In this paper the estimation of constrained states in nonlinear singular systems is addressed using an unscented recursive nonlinear dynamic data reconciliation with unknown inputs (URNDDR-UI) approach. It is known that the regular unscented recursive nonlinear dynamic data reconciliation (URNDDR) approach can reliably and accurately estimate nonlinear states with bounds and other constraints which are quite common in chemical processes. However, when there are arbitrary unknown inputs (e.g., deterministic disturbances which cannot be regarded as stable white noises) presented in the model and measurement equations, the regular URNDDR fails to cope with this case. In this regard, a recursive weighted least squares estimation (WLSE) is used in combination with the unscented transformation (UT) and nonlinear optimization (NO) methods to formulate the proposed URNDDR-UI approach whose major advantage lies in its capability of simultaneously estimating constrained states and unknown inputs. Simulation results demonstrate the efficiency of the proposed URNDDR-UI and its potential of applications to chemical processes.**

I. Introduction

The state estimation of singular systems / descriptor systems / implicit systems / differential-algebraic equations (DAE) (systems in which the differential and algebraic equations are coupled) have attracted enormous research efforts in the recent decades [1–3]. The most fundamental state estimation algorithm available for nonlinear singular systems is the extended Kalman filter (EKF) [4] due to its simpler implementation and less computational loads. Unfortunately, EKF has serious drawbacks in stability and accuracy which originates from linearizing the nonlinear differential-algebraic equations (DAEs) with the first-order Taylor series expansion. In addition, the formulations of Jacobians for the nonlinear equations consume considerable work, especially for high dimensional nonlinear singular systems. The unscented Kalman filter (UKF) [5, 6] approximates the nonlinearity at least to the second order with the unscented transformation (UT) method to provide more accurate and stable estimation than the EKF does. With the aid of a set of deterministic sigma points, the calculations for state covariance and Kalman gain matrices of UKF do not need the Jacobians. To this end, UKF is a better choice in the state estimation of nonlinear singular systems. Other nonlinear filtering approaches such as the particle filter (PF) [7] can deal with non-Gaussian case. However, increasing the size of particles of PF to improve its performance or reducing the size to relieve the computational load is still needed to be balanced.

In the state estimation of nonlinear singular systems, the physical meanings of the states frequently contradict their estimations. For instance, the compositions of components to be estimated in batch distillation operations should be positive physically, whilst they are sometimes negative mathematically due to multiple reasons including the linearization error of the nonlinear model, inaccurate initial conditions, multi-modal state probability density function, etc. To overcome this problem, the formulations handling the state constraints were presented in the literature [8, 9]. Among those approaches, the unscented recursive nonlinear dynamic data reconciliation (URNDDR) [10, 11] replaced the update step of UKF with a set of optimization problems for each sigma point to satisfy the constraints. Those URNDDR approaches are flexible to different natures of the constraints (equality/nonequality, convex/nonconvex, etc.) while inherit the advantages of UKF.

On the other hand, the presences of arbitrary unknown inputs could severely restrict the performances of the filtering approaches for nonlinear singular systems due to the high unbiasedness in the state estimation. As a result, the joint estimation of states and unknown inputs for the nonlinear singular systems has been studied for decades [1, 2]. However, to the best of the authors' knowledge, neither the case in which unknown inputs presented in the measurement equations nor the case dealing with the estimation of constrained states and unknown inputs is available in the open literature.

In this paper, an URNDDR-UI approach is proposed for the estimation of constrained state and unknown inputs in the model and measurement equations of nonlinear singular systems. This paper is organized as follows. Section II provides the formulation of RNDDR-UI which is the basis of the proposed URNDDR-UI. Section III presents the proposed URNDDR-UI. Section IV presents illustrative example to

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demonstrate the effectiveness of the URNDDR-UI approach. Section V concludes the paper.

II. The Formulation of RNDDR-UI

In [12], the EKF-UI approach was proposed for nonlinear regular systems with unknown inputs. In this paper, an EKF-based RNDDR approach is formulated following the similar route of EKF-UI to deal with the constrained states. Consider the following nonlinear singular system

$$\begin{aligned}&\dot{\mathbf{Z}}(t) = \mathbf{g}_c(\mathbf{Z}(t),\ \mathbf{X}(t),\ \mathbf{u}(t),\ \mathbf{u}^*(t)) + \mathbf{w}(t)\\ &\bar{\mathbf{g}}(\mathbf{Z}(t),\ \mathbf{X}(t)) = \mathbf{0}\\ &\mathbf{y}(t) = \mathbf{h}(\mathbf{Z}(t),\ \mathbf{X}(t),\ \mathbf{u}(t),\ \mathbf{u}^*(t)) + \mathbf{v}(t)\end{aligned} \tag{1}$$

where $\mathbf{g}_c$, $\bar{\mathbf{g}}$ and $\mathbf{h}_c$ denote n-, $\bar{m}$- and p-nonlinear continuous functions; $\mathbf{Z}(t)$ and $\mathbf{X}(t)$ denote the n-differential and m-algebraic state vectors, respectively; $\mathbf{u}(t)$ and $\mathbf{u}^*(t)$ denote the s-known input and r-unknown input vectors, respectively; $\mathbf{y}(t)$ denotes the p-measurement vector, and $\mathbf{w}(t)$ and $\mathbf{v}(t)$ denotes the continuous white noises. In this paper, the regularity and well-posedness [13] assumptions are held to guarantee unique solutions and finite variances of the states in the nonlinear singular system.

Eq.(1) can be further written as the following regular state space equations with constraints,

$$\begin{aligned}&\dot{\mathbf{Z}}(t) = \mathbf{g}_c(\mathbf{Z}(t),\ \bar{\mathbf{X}}(t),\ \mathbf{u}(t)) + \mathbf{w}(t)\\ &\bar{\mathbf{y}}(t) = \bar{\mathbf{h}}(\mathbf{Z}(t),\ \bar{\mathbf{X}}(t),\ \mathbf{u}(t)) + \bar{\mathbf{v}}(t)\\ &\mathbf{Z}_L \le \mathbf{Z}(t) \le \mathbf{Z}_U;\ \bar{\mathbf{X}}_L \le \bar{\mathbf{X}}(t) \le \bar{\mathbf{X}}_U\\ &\mathbf{f}_1(\mathbf{Z}(t),\ \hat{\bar{\mathbf{X}}}(t)) < \mathbf{0};\ \mathbf{f}_2(\mathbf{Z}(t),\ \bar{\mathbf{X}}(t)) = \mathbf{0}\end{aligned} \tag{2}$$

where $\bar{\mathbf{y}} = [\mathbf{y}^T\ \mathbf{0}_{1\times\bar{m}}]^T$, $\bar{\mathbf{h}} = [\mathbf{h}_c^T\ \bar{\mathbf{g}}^T]^T$, $\bar{\mathbf{X}} = [\mathbf{X}^T\ \mathbf{u}^{*T}]^T$ and $\bar{\mathbf{v}} = [\mathbf{v}^T\ \mathbf{0}_{1\times\bar{m}}]^T$, $\mathbf{Z}_L$ and $\bar{\mathbf{X}}_L$ are lower bounds for $\mathbf{Z}$ and $\bar{\mathbf{X}}$ respectively, $\mathbf{Z}_U$ and $\bar{\mathbf{X}}_U$ are upper bounds for $\mathbf{Z}$ and $\bar{\mathbf{X}}$ respectively, $\mathbf{f}_1$ and $\mathbf{f}_2$ are functions for inequality and equality constraints, respectively. It can been observed from Eq.(2) that the unknown inputs have been regarded as a part of the algebraic states of the nonlinear singular systems.

Substituting the first order approximation $\dot{\mathbf{Z}}(k\Delta t) = (\mathbf{Z}(k\Delta t) - \mathbf{Z}((k-1)\Delta t))/\Delta t$ into Eq.(2), the following nonlinear discrete state space equations can be obtained,

$$\mathbf{Z}_k = \mathbf{g}_{k-1} + \mathbf{w}_{k-1} \tag{3}$$

$$\bar{\mathbf{y}}_k = \bar{\mathbf{h}}_k + \bar{\mathbf{v}}_k \tag{4}$$

where

$$\mathbf{g}_{k-1} = \mathbf{Z}_{k-1} + \Delta t\ \mathbf{g}_c(\mathbf{Z}, \bar{\mathbf{X}}, \mathbf{u}, (k-1)\Delta t) \tag{5}$$

$$\bar{\mathbf{h}}_k = \bar{\mathbf{h}}(\mathbf{Z}_k, \bar{\mathbf{X}}_k, \mathbf{u}_k, k) \tag{6}$$

in which $\mathbf{Z}_k = \mathbf{Z}(k\Delta t)$ and $\mathbf{Z}_{k-1} = \mathbf{Z}((k-1)\Delta t)$, $\bar{\mathbf{X}}_k = \bar{\mathbf{X}}(k\Delta t)$ and $\bar{\mathbf{X}}_{k-1} = \bar{\mathbf{X}}((k-1)\Delta t)$; $\bar{\mathbf{y}}_k = \bar{\mathbf{y}}(k\Delta t)$; $\mathbf{u}_k = \mathbf{u}(k\Delta t)$; $\mathbf{u}_{k-1} = \mathbf{u}((k-1)\Delta t)$; $\mathbf{w}_{k-1} = \Delta t\ \mathbf{w}((k-1)\Delta t)$ and $\bar{\mathbf{v}}_k = \bar{\mathbf{v}}(k\Delta t)$ where $E[\mathbf{w}_{k-1}\mathbf{w}_{k-1}^T] = \mathbf{Q}_{k-1}$ and $E[\bar{\mathbf{v}}_k\bar{\mathbf{v}}_k^T] = \bar{\mathbf{R}}_k$, respectively. In the following, $\bar{\mathbf{R}}_k$ is assumed nonsingular (i.e., $\bar{\mathbf{v}} = [\mathbf{v}^T\ \tilde{\mathbf{v}}^T]^T$ where $\tilde{\mathbf{v}}$ are from the linearization errors of $\bar{\mathbf{g}}$).

The RNDDR-UI is proposed to solve the following problem: estimate states $\mathbf{Z}$ and $\bar{\mathbf{X}}$ under constraints at $t = k\Delta t$ denoted as $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$, respectively, given the observations ($\mathbf{y}_1$, $\mathbf{y}_2$, …, $\mathbf{y}_k$).

The RNDDR-UI is derived in the following (see [12]).

(i) Linearize the model and measurement equations with respect to the estimates of previous states

The nonlinear functions $\mathbf{g}_{k-1}$ in Eq.(5) and $\bar{\mathbf{h}}_k$ in Eq.(6) are linearized to give,

$$\begin{aligned}\mathbf{g}_{k-1} \approx\ &\hat{\mathbf{g}}_{k-1|k-1} + \mathbf{G}_{k-1|k-1}(\mathbf{Z}_{k-1} - \hat{\mathbf{Z}}_{k-1|k-1})\\ &+ \mathbf{B}_{k-1|k-1}(\bar{\mathbf{X}}_{k-1} - \hat{\bar{\mathbf{X}}}_{k-1|k-1})\end{aligned} \tag{7}$$

$$\bar{\mathbf{h}}_k \approx \hat{\bar{\mathbf{h}}}_{k|k-1} + \mathbf{H}_{k|k-1}(\mathbf{Z}_k - \hat{\mathbf{Z}}_{k|k-1}) + \mathbf{D}_{k|k-1}(\bar{\mathbf{X}}_k - \hat{\bar{\mathbf{X}}}_{k-1|k-1}) \tag{8}$$

where

$$\hat{\mathbf{g}}_{k-1|k-1} = \mathbf{g}(\hat{\mathbf{Z}}_{k-1|k-1}, \hat{\bar{\mathbf{X}}}_{k-1|k-1}, \mathbf{u}_{k-1}, k-1) \tag{9}$$

$$\hat{\bar{\mathbf{h}}}_{k|k-1} = \mathbf{h}(\hat{\mathbf{Z}}_{k|k-1}, \hat{\bar{\mathbf{X}}}_{k|k}, \mathbf{u}_k, k) \tag{10}$$

$$\mathbf{G}_{k-1|k-1} = \left[\partial\,\mathbf{g}_{k-1}/\partial\,\mathbf{Z}_{k-1}\right]_{\mathbf{Z}_{k-1}=\hat{\mathbf{Z}}_{k-1|k-1},\ \bar{\mathbf{X}}_{k-1}=\hat{\bar{\mathbf{X}}}_{k-1|k-1}} \tag{11}$$

$$\mathbf{B}_{k-1|k-1} = \left[\partial\,\mathbf{g}_{k-1}/\partial\,\bar{\mathbf{X}}_{k-1}\right]_{\mathbf{Z}_{k-1}=\hat{\mathbf{Z}}_{k-1|k-1},\ \bar{\mathbf{X}}_{k-1}=\hat{\bar{\mathbf{X}}}_{k-1|k-1}} \tag{12}$$

$$\mathbf{H}_{k|k-1} = \left[\partial\,\bar{\mathbf{h}}_k/\partial\,\mathbf{Z}_k\right]_{\mathbf{Z}_k=\hat{\mathbf{Z}}_{k|k-1},\ \bar{\mathbf{X}}_k=\hat{\bar{\mathbf{X}}}_{k|k}} \tag{13}$$

$$\mathbf{D}_{k|k-1} = \left[\partial\,\bar{\mathbf{h}}_k/\partial\,\bar{\mathbf{X}}_k\right]_{\mathbf{Z}_k=\hat{\mathbf{Z}}_{k|k-1},\ \bar{\mathbf{X}}_k=\hat{\bar{\mathbf{X}}}_{k|k}} \tag{14}$$

(ii) Minimize the linearized quadratic objective function to obtain the weighted least squares estimation of an extended state vector

The objective function of the summed square error between $\bar{\mathbf{y}}_i$ and $\bar{\mathbf{h}}_i$ (i = 1, 2, …, k) is given as follows

$$J_k = \bar{\mathbf{\Delta}}_k^T\ \mathbf{W}_k\ \bar{\mathbf{\Delta}}_k \tag{15}$$

where $\mathbf{W}_k$ is a $[(p+\bar{m})k\times(p+\bar{m})k]$ weighting matrix which is defined as the inverse of the covariance matrix for model and measurement noises; $\mathbf{\Delta}_i = \bar{\mathbf{y}}_i - \bar{\mathbf{h}}_i$ is a $(p+\bar{m})$-output error vector at $t = i\Delta t$ (i = 1, 2, …, k) and $\bar{\boldsymbol{\Delta}}_k = [\boldsymbol{\Delta}_1^T, \boldsymbol{\Delta}_2^T, \cdots, \boldsymbol{\Delta}_k^T]^T$ is a $(p+\bar{m})$k-vector. With the aid of the state transition relationship Eq.(3) and the linearized equations Eqs.(7)&(8), J_k in Eq.(15) becomes a linearized quadratic objective function of the extended state vector $\mathbf{Z}_{e,k} = [\mathbf{Z}_k^T \mid \bar{\mathbf{X}}_1^T \mid \bar{\mathbf{X}}_2^T \mid \cdots \mid \bar{\mathbf{X}}_k^T]^T$. Minimizing J_k with respect $\mathbf{Z}_{e,k}$ to obtain the weighted least square estimation (LSE) $\hat{\mathbf{Z}}_{e,k|k}$ of $\mathbf{Z}_{e,k}$ at $t = k\Delta t$ as follows (i.e. $\hat{\mathbf{Z}}_{e,k|k}$ satisfies $\left.\frac{\partial J_k}{\partial \mathbf{Z}_{e,k}}\right|_{\mathbf{Z}_{e,k}=\hat{\mathbf{Z}}_{e,k|k}} = \mathbf{0}$):

$$\hat{\mathbf{Z}}_{e,k|k} = \mathbf{P}_{e,k}[\mathbf{A}_{e,k}^T \mathbf{W}_k \mathbf{Y}_k];\ \mathbf{P}_{e,k} = [\mathbf{A}_{e,k}^T \mathbf{W}_k \mathbf{A}_{e,k}]^{-1} \quad (16)$$

where $\hat{\mathbf{Z}}_{e,k|k} = [\hat{\mathbf{Z}}_{k|k}^T \mid \hat{\bar{\mathbf{X}}}_{1|k}^T \mid \hat{\bar{\mathbf{X}}}_{2|k}^T \mid \cdots \mid \hat{\bar{\mathbf{X}}}_{k|k}^T]^T$, $\mathbf{Y}_k$ is a $(p+\bar{m})$k-known vector and $\mathbf{A}_{e,k}$ is a $[(p+\bar{m})k\times(n+k(m+r))]$ known matrix.

Though the final goal is to obtain the recursive estimates $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$, the recursive solution for the extended state vector $\hat{\mathbf{Z}}_{e,k|k}$ (the relationship between $\hat{\mathbf{Z}}_{e,k|k}$ at $t = k\Delta t$ and $\hat{\mathbf{Z}}_{e,k-1|k-1}$ at $t = (k-1)\Delta t$) should be derived first, i.e.,

$$\hat{\mathbf{Z}}_{e,k|k} = \begin{bmatrix} \bar{\mathbf{Z}}_{e,k} - \bar{\mathbf{P}}_{e,k}\tilde{\mathbf{H}}_k^T \bar{\mathbf{R}}_k^{-1} \mathbf{D}_{k|k-1} \hat{\bar{\mathbf{X}}}_{k|k} \\ \hline \hat{\bar{\mathbf{X}}}_{k|k} \end{bmatrix} \quad (17)$$

$$\tilde{\mathbf{H}}_k = [\mathbf{H}_{k|k-1} \mid \mathbf{0}_{(p+\bar{m})\times[(m+r)(k-1)]}] \quad (18)$$

where $\bar{\mathbf{Z}}_{e,k}$ is a $[n+(k-1)(m+r)]$-vector which is the function of $\hat{\mathbf{Z}}_{e,k-1|k-1}$, and $\bar{\mathbf{P}}_{e,k}$ is a $[(n+(k-1)(m+r))\times(n+(k-1)(m+r))]$ matrix with the information of $\mathbf{P}_{e,k-1} = [\mathbf{A}_{e,k-1}^T \mathbf{W}_{k-1} \mathbf{A}_{e,k-1}]^{-1}$.

(iii) Extract the Recursive $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$

It should be noted that the dimension of $\hat{\mathbf{Z}}_{e,k|k}$ (i.e., $[n+(k-1)(m+r)]$) will increase to infinity as the time instant k increases thus enlarging the computational load to infinity. To avoid this situation, the recursive solutions for $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$ should be extracted from Eq.(17) by partitioning $\hat{\mathbf{Z}}_{e,k|k}$ and $\hat{\mathbf{Z}}_{e,k-1|k-1}$ in Eq.(17) as follows:

$$\hat{\mathbf{Z}}_{e,k|k} = [\hat{\mathbf{Z}}_{k|k}^T \mid \hat{\mathbf{U}}_{k-1|k}^T \mid \hat{\bar{\mathbf{X}}}_{k|k}^T]^T \quad (19)$$

$$\hat{\mathbf{Z}}_{e,k-1|k-1} = [\hat{\mathbf{Z}}_{k-1|k-1}^T \mid \hat{\mathbf{U}}_{k-1|k-1}^T]^T \quad (20)$$

where $\hat{\mathbf{U}}_{k-1|k} = [\hat{\bar{\mathbf{X}}}_{1|k}^T \mid \hat{\bar{\mathbf{X}}}_{2|k}^T \mid \cdots \mid \hat{\bar{\mathbf{X}}}_{k-1|k}^T]^T$ and $\hat{\mathbf{U}}_{k-1|k-1} = [\hat{\bar{\mathbf{X}}}_{1|k-1}^T \mid \hat{\bar{\mathbf{X}}}_{2|k-1}^T \mid \cdots \mid \hat{\bar{\mathbf{X}}}_{k-1|k-1}^T]^T$ are both $[(k-1)(m+r)]$-vectors.

By substituting Eqs.(19)&(20) into Eq.(17) and operating a long and complex derivation procedure, the desirable recursive solutions for $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$ (RNDDR-UI) are obtained in the following.

<u>Step I: Prediction</u>

$$\hat{\mathbf{Z}}_{k|k-1} = \mathbf{g}(\hat{\mathbf{Z}}_{k-1|k-1}, \hat{\bar{\mathbf{X}}}_{k-1|k-1}, \mathbf{u}_{k-1}, k-1) \quad (21)$$

where $\hat{\mathbf{Z}}_{k-1|k-1}$ and $\hat{\bar{\mathbf{X}}}_{k-1|k-1}$ are differential and algebraic states at $t = (k-1)\Delta t$, respectively.

<u>Step II: Gain Matrices Computation</u>

The computations of the gain matrices for the differential and algebraic states at $t = k\Delta t$ ($\mathbf{K}_k$ and $\mathbf{S}_k$) are respectively given by

$$\mathbf{K}_k = \mathbf{P}_{\tilde{\mathbf{Z}}\tilde{\mathbf{y}}_k} \mathbf{P}_{\tilde{\mathbf{y}}_k}^{-1};\quad \mathbf{S}_k = \mathbf{P}_{\tilde{\mathbf{X}}_k} \quad (22)$$

where

$$\mathbf{P}_{\tilde{\mathbf{Z}}\tilde{\mathbf{y}}_k} = E[\tilde{\mathbf{Z}}_k \tilde{\mathbf{y}}_k^T];\ \mathbf{P}_{\tilde{\mathbf{y}}_k} = E[\tilde{\mathbf{y}}_k \tilde{\mathbf{y}}_k^T];\ \mathbf{P}_{\tilde{\mathbf{X}}_k} = E[\tilde{\mathbf{X}}_k \tilde{\mathbf{X}}_k^T] \quad (23)$$

in which

$$\tilde{\mathbf{Z}}_k = \mathbf{Z}_k - \hat{\mathbf{Z}}_{k|k-1};\ \tilde{\mathbf{y}}_k = \bar{\mathbf{y}}_k - \hat{\bar{\mathbf{y}}}_k;\ \tilde{\mathbf{X}}_k = \bar{\mathbf{X}}_k - \hat{\bar{\mathbf{X}}}_{k|k} \quad (24)$$

$$\bar{\mathbf{y}}_k = \bar{\mathbf{h}}(\mathbf{Z}_k, \mathbf{0}, \mathbf{u}_k, k);\ \hat{\bar{\mathbf{y}}}_k = \bar{\mathbf{h}}(\hat{\mathbf{Z}}_{k|k-1}, \mathbf{0}, \mathbf{u}_k, k) \quad (25)$$

The covariance matrices $\mathbf{P}_{\tilde{\mathbf{Z}}\tilde{\mathbf{y}}_k}$, $\mathbf{P}_{\tilde{\mathbf{y}}_k}$ and $\mathbf{P}_{\tilde{\mathbf{X}}_k}$ given in Eq.(23) for RNDDR-UI are realized by

$$\mathbf{P}_{\tilde{\mathbf{Z}}\tilde{\mathbf{y}}_k} = \mathbf{P}_{\tilde{\mathbf{Z}}} \mathbf{H}_{k|k-1}^T;\ \mathbf{P}_{\tilde{\mathbf{y}}_k} = \bar{\mathbf{R}}_k + \mathbf{H}_{k|k-1} \mathbf{P}_{\tilde{\mathbf{Z}}} \mathbf{H}_{k|k-1}^T \quad (26)$$

$$\mathbf{P}_{\tilde{\mathbf{X}}_k} = [\mathbf{D}_{k|k-1}^T \bar{\mathbf{R}}_k^{-1} (\mathbf{I} - \mathbf{H}_{k|k-1} \mathbf{K}_k) \mathbf{D}_{k|k-1}]^{-1} \quad (27)$$

in which

$$\mathbf{P}_{\tilde{\mathbf{Z}}_k} = E[\tilde{\mathbf{Z}}_k \tilde{\mathbf{Z}}_k^T] = \mathbf{G}_{k-1|k-1} \mathbf{P}_{\mathbf{Z}_{k-1}} \mathbf{G}_{k-1|k-1}^T + \mathbf{Q}_{k-1} \quad (28)$$

$$\mathbf{P}_{\mathbf{Z}_{k-1}} = \mathbf{E}[(\mathbf{Z}_{k-1} - \hat{\mathbf{Z}}_{k-1|k-1})(\mathbf{Z}_{k-1} - \hat{\mathbf{Z}}_{k-1|k-1})^T] \quad (29)$$

where and $\mathbf{Q}_{k-1}$ is the autocovariance function of the model noise process vector $\mathbf{w}_{k-1}$.

<u>Step III: Measurement Update</u>

Based on the previous studies [10, 11], the date reconciliation step for constrained states $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$ of nonlinear singular systems is implemented by minimizing the following objective function with respect to $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$

$$\begin{aligned} \bar{J}_k &= (\hat{\mathbf{Z}}_{k|k} - \hat{\mathbf{Z}}_{k|k-1})^T \mathbf{P}_{\tilde{\mathbf{Z}}_k}^{-1} (\hat{\mathbf{Z}}_{k|k} - \hat{\mathbf{Z}}_{k|k-1}) \\ &\quad + (\bar{\mathbf{y}}_k - \bar{\mathbf{h}}_k)^T \mathbf{R}_k^{-1} (\bar{\mathbf{y}}_k - \bar{\mathbf{h}}_k) \end{aligned} \quad (30)$$

Subject to the following constraints:

$$\mathbf{Z}_L \le \hat{\mathbf{Z}}_{k|k} \le \mathbf{Z}_U;\quad \bar{\mathbf{X}}_L \le \hat{\bar{\mathbf{X}}}_{k|k} \le \bar{\mathbf{X}}_U$$

$$\mathbf{f}_1(\hat{\mathbf{Z}}_{k|k}, \hat{\bar{\mathbf{X}}}_{k|k}) \le \mathbf{0};\quad \mathbf{f}_2(\hat{\mathbf{Z}}_{k|k}, \hat{\bar{\mathbf{X}}}_{k|k}) = \mathbf{0} \tag{31}$$

in which $\hat{\mathbf{Z}}_{k|k-1}$ and $\mathbf{P}_{\tilde{\mathbf{Z}}_k}$ are given by Eqs.(21)&(28) respectively, $\bar{\mathbf{y}}_k$, $\bar{\mathbf{h}}_k$, and $\mathbf{R}_k$ are defined by Eqs.(5)&(6). The posterior state covariance matrix $\mathbf{P}_{\mathbf{Z}_k}$ is given by

$$\mathbf{P}_{\mathbf{Z}_k} = \mathbf{P}_{\tilde{\mathbf{Z}}_k} - \mathbf{K}_k\mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} + \mathbf{K}_k\mathbf{P}_{\tilde{\mathbf{y}}^*_k}\bar{\mathbf{R}}_k^{-1}\mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} + \mathbf{K}_k\mathbf{P}_{\tilde{\mathbf{y}}^*_k}(\mathbf{P}_{\tilde{\mathbf{y}}_k}^{-1} - \bar{\mathbf{R}}_k^{-1})\mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} \tag{32}$$

in which

$$\mathbf{P}_{\bar{\mathbf{X}}\tilde{\mathbf{y}}^*_k} = \mathrm{E}[\bar{\mathbf{X}}_k\tilde{\mathbf{y}}_k^{*T}];\quad \mathbf{P}_{\tilde{\mathbf{y}}^*_k} = \mathrm{E}[\tilde{\mathbf{y}}^*_k\tilde{\mathbf{y}}_k^{*T}];\quad \mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} = \mathrm{E}[\tilde{\mathbf{y}}_k\tilde{\mathbf{Z}}_k^T] \tag{33}$$

where

$$\tilde{\mathbf{y}}^*_k = \bar{\mathbf{h}}(\mathbf{0}, \bar{\mathbf{X}}_k, \mathbf{u}_k, k) - \bar{\mathbf{h}}(\mathbf{0}, \hat{\bar{\mathbf{X}}}_{k|k}, \mathbf{u}_k, k) \tag{34}$$

For the RNDDR-UI,

$$\mathbf{P}_{\bar{\mathbf{X}}\tilde{\mathbf{y}}^*_k} = \mathbf{S}_k\mathbf{D}_{k|k-1}^T;\quad \mathbf{P}_{\tilde{\mathbf{y}}_k}^{-1} = \bar{\mathbf{R}}_k^{-1}(\mathbf{I} - \mathbf{H}_{k|k-1}\mathbf{K}_k);$$

$$\mathbf{P}_{\tilde{\mathbf{y}}^*_k} = \mathbf{D}_{k|k-1}\mathbf{S}_k\mathbf{D}_{k|k-1}^T;\quad \mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} = \mathbf{H}_{k|k-1}\mathbf{P}_{\mathbf{Z}_{k-1}} \tag{35}$$

Eqs. (21)-(35) give the solutions of the proposed RNDDR-UI. The unknown inputs in the model and measurement equations can be estimated together with $\hat{\mathbf{Z}}_{k|k}$ by being regarded as a part of $\hat{\bar{\mathbf{X}}}_{k|k}$.

Remark 1: When m = 0 and r = 0 (m and r are the dimensions of the algebraic states $\mathbf{X}(t)$ and unknown inputs $\mathbf{u}^*(t)$, respectively) and the constraints in Eq.(31) are off, the RNDDR-UI reduces to the traditional extended Kalman filter (EKF) approach.

Remark 2: The existence of the unique estimation solutions for Eqs. (21)-(35) is equivalent to the invertibility of the matrix $\mathbf{P}_{e,k} = [\mathbf{A}_{e,k}^T\mathbf{W}_k\mathbf{A}_{e,k}]^{-1}$ in Eq.(16), i.e., the full column rank of the matrix $\mathbf{A}_{e,k}$, which is correlated with the dimension of the measurement vector, the structure and number of the algebraic states, etc. Based on the LSE property, the necessary condition of the proposed RNDDR-UI which can be used for fast checking is given: the dimension of $\bar{\mathbf{y}}_k$ (i.e., p + $\bar{m}$) is greater than the dimension of $\bar{\mathbf{X}}$ (i.e., m + r), which means, the number of output equations should be greater than the number of unknowns to be estimated by LSE.

Remark 3: Although the RNDDR-UI given by Eqs.(21)-(35) is derived based on the first order approximation of the nonlinear singular system and the LSE formulation, the covariance matrices in the solutions (see Eqs. (26)-(28) & (35)) are with the stochastic meanings thus not being restricted to LSE implementation. This fact is useful for the formulation of the next section.

III. THE FORMULATION OF URNDDR-UI

Though the RNDDR-UI proposed in Section II is able to deal with the estimation of states and unknown inputs for nonlinear singular systems, two drawbacks encumber its applications in the reality: (i) it is derived with the similar route of the regular EKF, as a result, it also inherits the serious accuracy and stability problem of the regular EKF, which has already stimulated the development of more advanced nonlinear filtering approaches (see the literature in Section I); (ii) it can not handle the constrained states which are usual in engineering systems. Inspired by the successful combination of the unscented transformation (UT) [5 ,6] and the RNDDR [10] which result in the URNDDR [11], a unscented recursive nonlinear dynamic data reconciliation with unknown inputs (URNDDR-UI) approach is formulated in this section by applying the UT method to the RNDDR-UI proposed in Section II.

<u>Step I: Sigma points calculation at $t = k\Delta t$</u>

Given $\hat{\mathbf{Z}}_{k-1|k-1}$, $\hat{\bar{\mathbf{X}}}_{k-1|k-1}$, $\mathbf{P}_{\mathbf{Z}_{k-1}}$ and $\mathbf{S}_{k-1}$ (the quantities at $t = (k-1)\Delta t$), the sigma points are calculated by

$$\chi_{0,k-1|k-1} = \hat{\mathbf{Z}}_{k-1|k-1};\quad \boldsymbol{\mu}_{0,k-1|k-2} = \hat{\bar{\mathbf{X}}}_{k-1|k-1}$$

$$\chi_{i,k-1|k-1} = \hat{\mathbf{Z}}_{k-1|k-1} + \left(\sqrt{(n+\lambda_1)\mathbf{P}_{\mathbf{Z}_{k-1}}}\right)_i,\quad i = 1, \ldots, n$$

$$\chi_{i,k-1|k-1} = \hat{\mathbf{Z}}_{k-1|k-1} - \left(\sqrt{(n+\lambda_1)\mathbf{P}_{\mathbf{Z}_{k-1}}}\right)_i,\quad i = n+1, \ldots, 2n$$

$$\boldsymbol{\mu}_{j,k-1|k-1} = \hat{\bar{\mathbf{X}}}_{k-1|k-1} + \left(\sqrt{(r+\lambda_2)\mathbf{S}_{k-1}}\right)_j,\quad j = 1, \ldots, m+r$$

$$\boldsymbol{\mu}_{j,k-1|k-1} = \hat{\bar{\mathbf{X}}}_{k-1|k-1} - \left(\sqrt{(r+\lambda_2)\mathbf{S}_{k-1}}\right)_j,\quad j = m+r+1, \ldots, 2(m+r) \tag{36}$$

in which $(\sqrt{\mathbf{A}})_i$ and $(\sqrt{\mathbf{B}})_j$ denote the *i*th and *j*th columns of the matrix square roots $\sqrt{\mathbf{A}}$ and $\sqrt{\mathbf{B}}$, respectively. The weights are calculated by

$$W_0^{(Z)} = \frac{\lambda_1}{n+\lambda_1};\quad W_0^{(\bar{X})} = \frac{\lambda_2}{r+\lambda_2}$$

$$W_0^{(CZ)} = \frac{\lambda_1}{n+\lambda_1} + 1 - \alpha_1^2 + \beta_1;\quad W_0^{(C\bar{X})} = \frac{\lambda_2}{r+\lambda_2} + 1 - \alpha_2^2 + \beta_2$$

$$W_i^{(Z)} = W_i^{(CZ)} = \frac{1}{2(n+\lambda_1)},\quad i = 1, \ldots, 2n$$

$$W_j^{(\bar{X})} = W_j^{(C\bar{X})} = \frac{1}{2(r+\lambda_2)},\quad i = 1, \ldots, 2(m+r) \tag{37}$$

where $\lambda_1 = \alpha_1^2(n+\kappa_1) - n$, $\lambda_2 = \alpha_2^2(m+r+\kappa_2) - (m+r)$, β_1, β_2, κ_1, $\kappa_2 \ge 0$ (default $\kappa_1 = \kappa_2 = 0$, $\beta_1 = \beta_2 = 2$), $0 \le \alpha_1, \alpha_2 \le 1$.

<u>Step II: Prediction</u>

By feeding sigma points through the nonlinear DAE system in Eq. (1), it is obtained (here the predicted unknown inputs are assumed equal to their estimation at $t=(k-1)\Delta t$)

$$\hat{\chi}_{i,k|k-1} = \mathbf{g}\,(\chi_{i,k-1|k-1}, \hat{\bar{\mathbf{X}}}_{k-1|k-1}, \mathbf{u}_{k-1}, k-1)$$

$$\hat{\boldsymbol{\mu}}_{j,k|k-1} = \boldsymbol{\mu}_{j,k-1|k-1};\ \gamma_{i,k|k-1} = \bar{\mathbf{h}}(\hat{\chi}_{i,k|k-1}, \hat{\bar{\mathbf{X}}}_{i,k|k-1}, \mathbf{u}_k, k)$$

$$i = 0, \ldots, 2n;\ j = 0, \ldots, 2(m+r) \qquad (38)$$

the predicted means are computed as follows

$$\hat{\mathbf{Z}}_{k|k-1} = \sum_{i=0}^{2n} W_i^{(Z)} \hat{\chi}_{i,k|k-1};\ \hat{\bar{\mathbf{X}}}_{k|k-1} = \sum_{j=0}^{2(m+r)} W_j^{(\bar{X})} \hat{\bar{\mathbf{X}}}_{i,k|k-1}$$

$$\hat{\bar{\mathbf{h}}}_{k|k-1} = \sum_{i=0}^{2n} W_i^{(Z)} \hat{\gamma}_{i,k|k-1} \qquad (39)$$

The corresponding predictions are computed by:

$$\bar{\chi}_{i,k|k-1} = \mathbf{g}\,(\chi_{i,k-1|k-1}, \hat{\bar{\mathbf{X}}}_{k-1|k-1}, \mathbf{u}_{k-1}, k-1) \qquad (40)$$

$$\bar{\gamma}_{i,k|k-1} = \bar{\mathbf{h}}(\bar{\chi}_{i,k|k-1}, \mathbf{0}, \mathbf{u}_k, k);\ i = 0, \ldots, 2n \qquad (41)$$

the predicted means are computed as follows

$$\hat{\bar{\mathbf{Z}}}_{k|k-1} = \sum_{i=0}^{2n} W_i^{(Z)} \bar{\chi}_{i,k|k-1};\ \hat{\bar{\mathbf{y}}}_k = \sum_{i=0}^{2n} W_i^{(Z)} \bar{\gamma}_{i,k|k-1} \qquad (42)$$

$$\gamma^*_{j,k|k-1} = \bar{\mathbf{h}}(\mathbf{0}, \boldsymbol{\mu}_{j,k-1|k-1}, \mathbf{u}_k, k);\quad j = 0, \ldots, 2(m+r) \qquad (43)$$

the predicted means are computed as follows

$$\gamma^*_{k|k-1} = \sum_{i=0}^{2(m+r)} W_i^{(\bar{X})} \gamma^*_{j,k|k-1} \qquad (44)$$

<u>Step III: Gain Matrices Computation</u>

The gain matrices $\mathbf{K}_k$ and $\mathbf{S}_k$ are computed by Eq.(22), in which

$$\mathbf{P}_{\tilde{\mathbf{X}}_k} = \sum_{j=0}^{2(m+r)} W_j^{(C\bar{X})} [\hat{\boldsymbol{\mu}}_{j,k|k-1} - \hat{\boldsymbol{\mu}}_{k|k-1}][\hat{\boldsymbol{\mu}}_{j,k|k-1} - \hat{\boldsymbol{\mu}}_{k|k-1}]^T \qquad (45)$$

$$\mathbf{P}_{\tilde{\mathbf{y}}_k} = \sum_{i=0}^{2n} W_i^{(CZ)} [\bar{\gamma}_{i,k|k-1} - \hat{\bar{\mathbf{y}}}_k][\bar{\gamma}_{i,k|k-1} - \hat{\bar{\mathbf{y}}}_k]^T \qquad (46)$$

$$\mathbf{P}_{\tilde{\mathbf{Z}}\tilde{\mathbf{y}}_k} = \sum_{i=0}^{2n} W_i^{(CZ)} [\bar{\chi}_{i,k|k-1} - \hat{\bar{\mathbf{Z}}}_{k|k-1}][\bar{\gamma}_{i,k|k-1} - \hat{\bar{\mathbf{y}}}_k]^T \qquad (47)$$

$$\mathbf{P}_{\tilde{\mathbf{y}}\tilde{\mathbf{Z}}_k} = \sum_{i=0}^{2n} W_i^{(CZ)} [\bar{\gamma}_{i,k|k-1} - \hat{\bar{\mathbf{y}}}_k][\bar{\chi}_{i,k|k-1} - \hat{\bar{\mathbf{Z}}}_{k|k-1}]^T \qquad (48)$$

<u>Step IV: Measurement Update</u>

The estimated differential and algebraic states $\hat{\mathbf{Z}}_{k|k}$ and $\hat{\bar{\mathbf{X}}}_{k|k}$, and the state error covariance matrix $\mathbf{P}_{\mathbf{Z}_k}$ are computed by Eqs.(30)-(32) in which minimizing the following objective function with respect to $\bar{\chi}_{i,k|k}$ and $\hat{\bar{\mathbf{X}}}_{i,k|k}$

$$J_{i,k} = (\bar{\chi}_{i,k|k} - \bar{\chi}_{i,k|k-1})^T \mathbf{P}^{-1}_{\tilde{\mathbf{Z}}_k} (\bar{\chi}_{i,k|k} - \bar{\chi}_{i,k|k-1}) + (\bar{\mathbf{y}}_k - \tilde{\bar{\mathbf{h}}}_k)^T \mathbf{R}_k^{-1} (\bar{\mathbf{y}}_k - \tilde{\bar{\mathbf{h}}}_k) \qquad (49)$$

subject to the following constraints:

$$\mathbf{Z}_L \le \bar{\chi}_{i,k|k} \le \mathbf{Z}_U;\ \bar{\mathbf{X}}_L \le \hat{\bar{\mathbf{X}}}_{i,k|k} \le \bar{\mathbf{X}}_U$$

$$\mathbf{f}_1(\bar{\chi}_{i,k|k}, \hat{\bar{\mathbf{X}}}_{k|k}) \le \mathbf{0};\ \mathbf{f}_2(\bar{\chi}_{i,k|k}, \hat{\bar{\mathbf{X}}}_{k|k}) = \mathbf{0} \qquad (50)$$

$$\mathbf{P}_{\tilde{\mathbf{X}}\tilde{\mathbf{y}}^*_k} = \sum_{j=0}^{2(m+r)} W_j^{(C\bar{X})} [\hat{\boldsymbol{\mu}}_{j,k|k-1} - \hat{\boldsymbol{\mu}}_{k|k-1}][\gamma^*_{j,k|k-1} - \gamma^*_{k|k-1}]^T \qquad (51)$$

$$\mathbf{P}_{\tilde{\mathbf{y}}^*_k} = \sum_{j=0}^{2(m+r)} W_j^{(C\bar{X})} [\gamma^*_{j,k|k-1} - \gamma^*_{k|k-1}][\gamma^*_{j,k|k-1} - \gamma^*_{k|k-1}]^T \qquad (52)$$

$$\mathbf{P}_{\tilde{\mathbf{Z}}_k} = \sum_{i=0}^{2n} W_i^{(CZ)} [\bar{\chi}_{i,k|k-1} - \hat{\bar{\mathbf{Z}}}_{k|k-1}][\bar{\chi}_{i,k|k-1} - \hat{\bar{\mathbf{Z}}}_{k|k-1}]^T \qquad (53)$$

In above, Eqs.(36)-(53) give the proposed URNDDR-UI approach. When the constraints in Eq.(50) are off, the URNDDR-UI reduces to the UKF-UI, which is an UKF for unconstrained states and unknown inputs.

IV. An Illustrative Example

In this section, a semi-explicit nonlinear singular system with index 1 [14] is given to verify the URNDDR-UI approach. The differential equations are described by

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{a}_1 \\ \dot{a}_2 \\ \dot{a}_3 \end{bmatrix} = \begin{bmatrix} -4\times10^{-2} a_1 + a_2 \cdot a_3 + f \\ 4\times10^{-2} a_1 - a_2 \cdot a_3 - 3\times10^{-1} a_2^2 \\ a_1 + 1\times10^{-4} a_2 + a_3 - 1 \end{bmatrix} \qquad (54)$$

which is subject to the constraints $a_2 \ge 0$ in which a_1, a_2 and a_3 are the time-dependent variables, f is time-dependent arbitrary disturbance in the process model. Let the differential and algebraic states be chosen as $\mathbf{Z} = [z_1 \quad z_2]^T = [a_1 \quad a_2]^T$ and $\mathbf{X} = x_1 = a_3$, respectively, and the unknown input $u^* = f$. The state space model of the nonlinear singular systems in Eq.(1) is given by

$$\mathbf{g}_c = \begin{bmatrix} -4\times10^{-2} z_1 + z_2 \cdot x_1 + u^* \\ 4\times10^{-2} z_1 - z_2 \cdot x_1 - 3\times10^{-1} z_2^2 \end{bmatrix};$$

$$\bar{\mathbf{g}} = z_1 + 1\times10^{-4} z_2 + x_1 - 1 \qquad (55)$$

The measurement equations are given by

$$\mathbf{h} = \begin{bmatrix} z_1 + u^* \\ z_1 + 2z_2 \end{bmatrix} \qquad (56)$$

The simulation procedure with initial values $a_1 = 1$, $a_2 = 0$, $a_3 = 0$ and $u^*(t) = f(t) = 0.02t$ runs for 100 seconds by using MATLAB ordinary differential equations solver 'ode15s'. The process noises are assumed as Gaussian noises with zero mean and standard deviation 0.05 and the measurements with sampling interval Δt = 0.05 sec.) and the differential states z_1 and z_2 are polluted by Gaussian noises (zero mean and standard deviation 0.2).

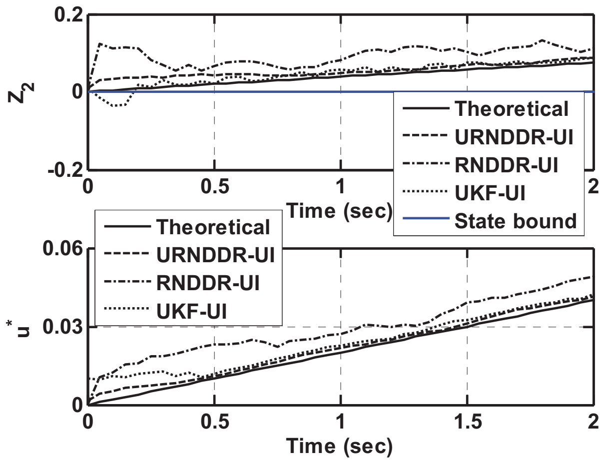

Fig.1. Estimated state z_2 and unknown input $\mathbf{u}^*$ with URNDDR-UI, RNDDR-UI and UKF-UI approaches.

Unknown quantities to be estimated by the proposed URNDDR-UI approach are: (i) the state vectors $\mathbf{Z}_k$ and $\mathbf{X}_k$; and (ii) the unknown input u_k^*. The initial states for the estimation are $\mathbf{Z}_0 = [0.9 \quad 0.01]^T$ and the initial covariance matrix are defined as $\mathbf{P}_{\mathbf{Z}_0}$ = (2×2) diagonal matrix = diag $\{10^{-2},\ 10^{-2}\}$.

Based on the URNDDR-UI approach given by Eqs. (36)-(53), the states and unknown inputs are estimated simultaneously. Due to space limit, only the estimation results of z_2 and unknown input u^* during the first 2 seconds are presented in Fig.1. To demonstrate the advantage of the proposed URNDDR-UI, the initial condition for z_2 (i.e., 0.01) is close to lower zero-bound. For comparison, the RNDDR-UI approach and UKF-UI (see the end of Section III for description) are also implemented.

It can be seen from Fig.1 that during the initial stage where the zero-bound constraint is obvious, the estimated z_2 with the proposed URNDDR-UI and RNDDR-UI keep both non-negative, whilst the one estimated with UKF-UI becomes negative at some time instants. This verifies the effectiveness of the constrained optimization in the former two approaches. During the stage where the state constraint is neglected, the estimation with UKF-UI and URNDDR-UI are similar and they are much better than the one of RNDDR-UI. This reveals the merit of the unscented transformation (UT) used in UKF-UI and URNDDR-UI.

In summary, the illustrative example shows that the proposed URNDDR-UI have the advantages over EKF-UI [12], RNDDR [10] and UKF [5].

V. Conclusions

In this paper, an URNDDR-UI approach is formulated on the basis of the EKF-UI [12], RNDDR [10] and UKF [5] to estimate the constrained states and unknown inputs of nonlinear singular systems. The illustrative example demonstrates the advantage of the proposed URNDDR approach. In future, the proposed URNDDR-UI will be extended to practical nonlinear singular systems within the engineering scope.

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